

=> fil hcap
FILE 'HCAPLUS' ENTERED AT 15:25:55 ON 16 JAN 2007
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FILE COVERS 1907 - 16 Jan 2007 VOL 146 ISS 4
FILE LAST UPDATED: 15 Jan 2007 (20070115/ED)

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=> s 151
L58 1 L51

=> s 152
L59 3 L52

=> s 153
L60 4 L53

=> fil hcap
FILE 'HCAPLUS' ENTERED AT 15:26:16 ON 16 JAN 2007
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FILE COVERS 1907 - 16 Jan 2007 VOL 146 ISS 4
FILE LAST UPDATED: 15 Jan 2007 (20070115/ED)

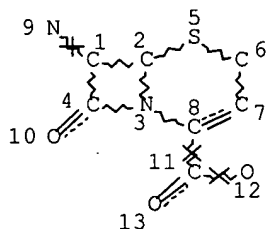
New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que 158

L1

STR



NODE ATTRIBUTES:

CONNECT IS M3 RC AT 7

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

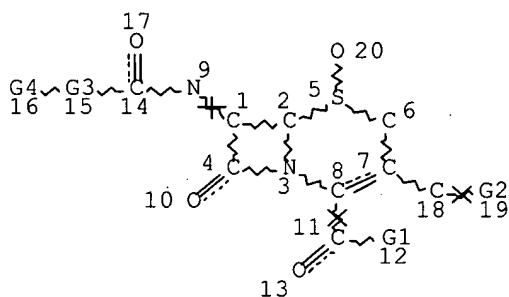
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

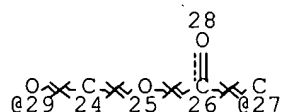
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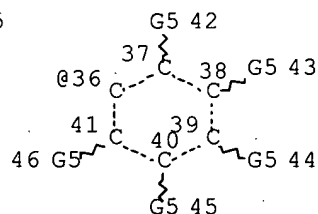
L40 STR



O @21

O ~ Ak
@22 23CH ~ Me
@30 31Me ~ C ~ Me
32 ~ @33 34

Hy @35



VAR G1=21/22/29/27

VAR G2=C/N

VAR G3=CH2/30/33

VAR G4=CN/35/36

VAR G5=H/ME

NODE ATTRIBUTES:

CONNECT IS M3 RC AT 7

CONNECT IS E1 RC AT 21

CONNECT IS E1 RC AT 23

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS X5 C AT 23
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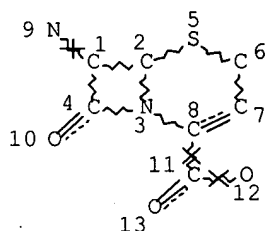
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 NUMBER OF NODES IS 46

STEREO ATTRIBUTES: NONE

L42 40 SEA FILE=REGISTRY SUB=L3 SSS FUL L40
 L51 1 SEA FILE=REGISTRY ABB=ON PLU=ON L42 AND OC5-C6-C6/ES
 L58 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L51

=> d que 159

L1 STR

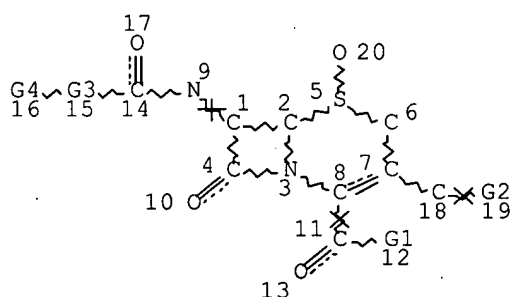


NODE ATTRIBUTES:
 CONNECT IS M3 RC AT 7
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

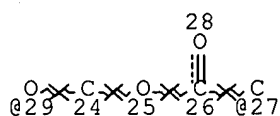
L3 81306 SEA FILE=REGISTRY SSS FUL L1
 L40 STR



O @21

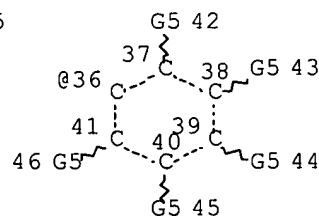
O~Ak
 @22 23

CH~Me
 @30 31



Me~C~Me
 32 @33 34

Hy @35



VAR G1=21/22/29/27

VAR G2=C/N

VAR G3=CH2/30/33

VAR G4=CN/35/36

VAR G5=H/ME

NODE ATTRIBUTES:

CONNECT IS M3 RC AT 7

CONNECT IS E1 RC AT 21

CONNECT IS E1 RC AT 23

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS X5 C AT 23

ECOUNT IS E4 C E1 S AT 35

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 46

STEREO ATTRIBUTES: NONE

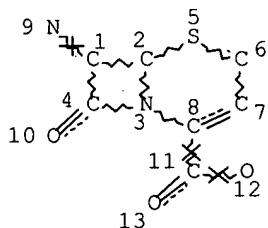
L42 40 SEA FILE=REGISTRY SUB=L3 SSS FUL L40

L52 2 SEA FILE=REGISTRY ABB=ON PLU=ON L42 AND OC5-C6/ES

L59 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L52

=> d que 160

L1 STR



NODE ATTRIBUTES:

CONNECT IS M3 RC AT 7

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

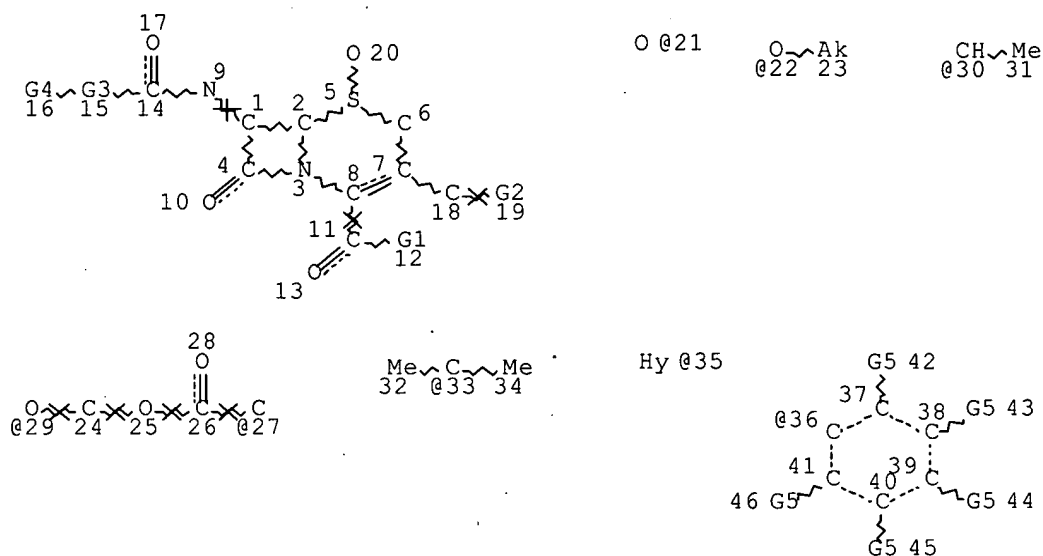
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L3 81306 SEA FILE=REGISTRY SSS FUL L1

L40 STR



VAR G1=21/22/29/27

VAR G2=C/N

VAR G3=CH2/30/33

VAR G4=CN/35/36

VAR G5=H/ME

NODE ATTRIBUTES:

CONNECT IS M3 RC AT 7

CONNECT IS E1 RC AT 21

CONNECT IS E1 RC AT 23

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS X5 C AT 23

ECOUNT IS E4 C E1 S AT 35

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 46

STEREO ATTRIBUTES: NONE

L42 40 SEA FILE=REGISTRY SUB=L3 SSS FUL L40

L53 5 SEA FILE=REGISTRY ABB=ON PLU=ON L42 AND NC2OC2-C6-C6/ES

L60 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L53

=> s 158-60

L61 6 (L58 OR L59 OR L60)

=> d l61 ibib abs hitstr tot

L61 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:571011 HCAPLUS Full-text

DOCUMENT NUMBER: 143:93614

TITLE: In vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery

INVENTOR(S): Graham, Ronald J.; Sekar, Michael; Barbisin, Maura

PATENT ASSIGNEE(S): Applera Corporation, USA

SOURCE: PCT Int. Appl., 54 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005059163	A2	20050630	WO 2004-US42639	20041215
WO 2005059163	A3	20051229		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005244907	A1	20051103	US 2004-14447	20041215
EP 1704244	A2	20060927	EP 2004-814782	20041215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
PRIORITY APPLN. INFO.:			US 2003-529953P	P 20031215
			US 2004-542425P	P 20040206
			WO 2004-US42639	W 20041215

AB The present disclosure relates to methods for detecting an activity of one or more enzymes in a cell. In some embodiments, a cell is contacted with a liposome containing a substrate capable of producing a detectable light signal when acted upon by the enzyme, and detecting the amount of a light signal in the cell, wherein the amount indicates a level of the enzyme activity in the cell. Encapsulation in a liposome facilitates intracellular delivery of substrate. The methods can be used in screening agents that can inhibit or activate an enzyme activity. The methods can also be used in various downstream assays such the detection of interactions between intracellular proteins, screening for variants of an enzyme, and detection of various diseases. Comps. and kits for carrying out the various methods are also provided. These results show that liposomes containing a substrate capable of generating a fluorescent signal when acted on by β -galactosidase can be used to detect activity of this enzyme in cells and can be used to determine the presence or absence of this activity in various cell types.

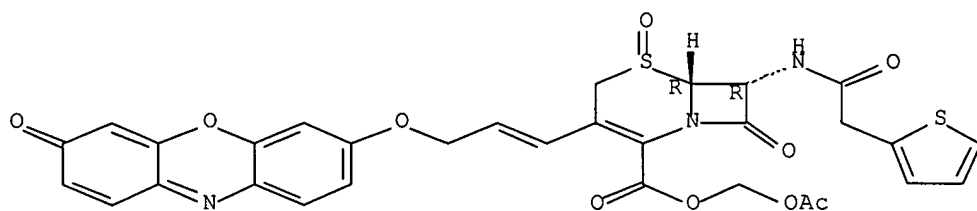
IT 452280-31-8 609812-89-7, 8-Oxo-3-[3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-[(phenylacetyl)amino]-5-oxide (6R,7R)-(9CI)

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (in vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery)

RN 452280-31-8 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 8-oxo-3-[3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, (acetyloxy)methyl ester, 5-oxide, (6R,7R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.

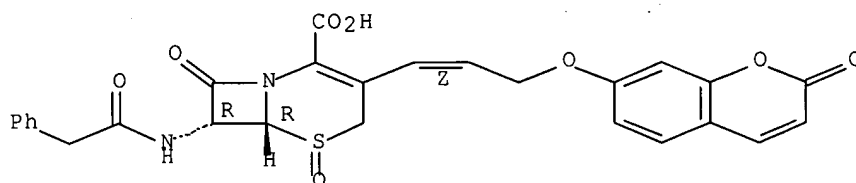


RN 609812-89-7 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
8-oxo-3-[(1Z)-3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-
[(phenylacetyl)amino]-, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L61 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:474830 HCAPLUS Full-text

DOCUMENT NUMBER: 143:22126

TITLE: Fluorogenic β -lactamase substrate containing a phenolic dye and vinyllogous cephalosporin, and use for monitoring β -lactamase reporter gene expression

INVENTOR(S): Tsien, Roger Y.; Rao, Jianghong

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 40 pp., Cont.-in-part of U.S. Ser. No. 44,486.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005118669	A1	20050602	US 2004-884019	20040702
US 2003003526	A1	20030102	US 2002-44486	20020111
US 2005181469	A1	20050818	US 2005-93399	20050329
WO 2006085978	A2	20060817	WO 2005-US23947	20050630

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF,
 CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM,
 KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG,
 KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:

US 2001-261313P P 20010112

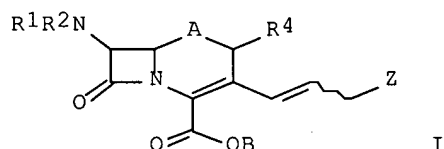
US 2002-44486 A2 20020111

US 2004-884019 A 20040702

OTHER SOURCE(S):

MARPAT 143:22126

GI



AB Provided are fluorescent substrates for β -lactamases having the general formula I ($R_1, R_2 = H$, benzyl, 2-thienylmethyl, cyanomethyl; $B = H$, physiol. acceptable salts or metal, ester groups, ammonium cations, $-\text{CHR}_5\text{OCO}(\text{CH}_2)_n\text{CH}_3$, $-\text{CHR}_5\text{OCOC}(\text{CH}_3)_3$, acylthiomethyl, acyloxy- α -benzyl, δ -butyrolactonyl, methoxycarbonyloxymethyl, Ph, methylsulphinylmethyl, δ -morpholinoethyl, dialkylaminoethyl, dialkylaminocarbonyloxymethyl; $R_4, R_5 = H$, lower alkyl; $A = S$, O , SO , SO_2 , CH_2 ; $Z =$ a donor fluorescent moiety that links to the lactam-containing group' $n = 0-10$). A new class of small fluorogenic substrates that work by releasing a phenolate from a vinyllogous cephalosporin is reported. The β -lactam ring is cleaved by a β -lactamase enzyme effective to free a fluorophore. Methods of assaying β -lactamase activity and monitoring expression in systems using beta-lactamase as a reporter gene are also disclosed.

IT 852671-27-3P 852671-28-4P 852671-29-5P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

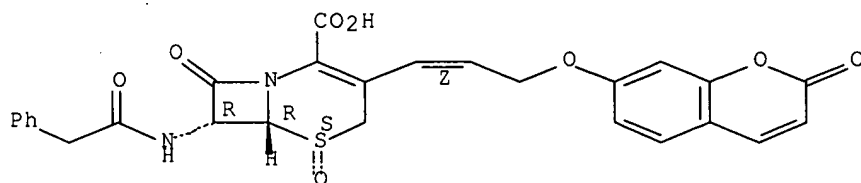
(fluorogenic β -lactamase substrate containing phenolic dye and vinyllogous cephalosporin, and use for monitoring β -lactamase reporter gene expression)

RN 852671-27-3 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 8-oxo-3-[(1Z)-3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-
 [(phenylacetyl)amino]-, 5-oxide, (5S,6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

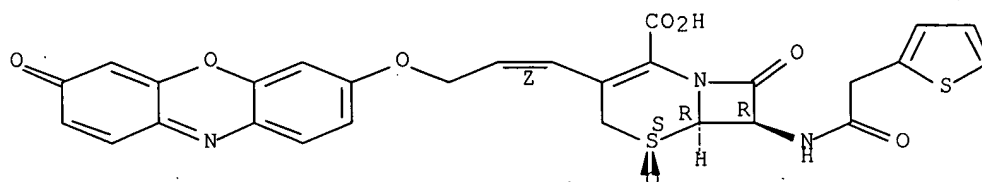


RN 852671-28-4 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, 5-oxide, (5S,6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

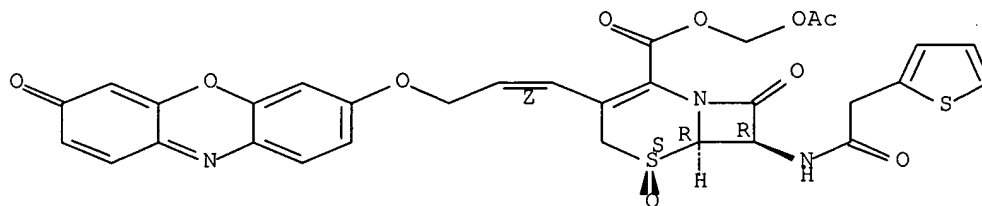


RN 852671-29-5 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, (acetyloxy)methyl ester, 5-oxide, (5S,6R,7R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L61 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:239156 HCAPLUS Full-text

DOCUMENT NUMBER: 142:312727

TITLE: Fluorescent probe used for hydrolase assay

INVENTOR(S): Nagano, Tetsuo; Kamiya, Mako; Urano, Yasuteru

PATENT ASSIGNEE(S): Daiichi Pure Chemicals Co., Ltd., Japan

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

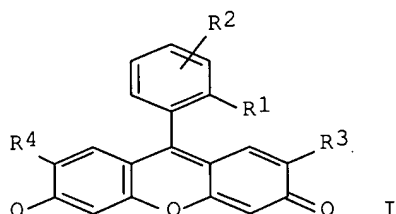
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005024049	A1	20050317	WO 2004-JP13185	20040903
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,				

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 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1674579 A1 20060628 EP 2004-772924 20040903
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

PRIORITY APPLN. INFO.: JP 2003-314041 A 20030905
 WO 2004-JP13185 W 20040903

OTHER SOURCE(S): MARPAT 142:312727
 GI



AB A novel fluorescent probe is provided, which is represented by the following formula (I), and is utilized for a fluorescence assay of a hydrolase. In the formula I, R1 represents a hydrogen atom, a carboxy group or a monovalent substituent other than a sulfonate group; R2 represents a hydrogen atom or a monovalent substituent; R3 and R4 each independently represents a hydrogen atom or a halogen atom; and R5 represents a monovalent group which is cleaved upon contact with a substance to be detected; provided that the combination of R1 and R2 is selected so that the benzene ring to which R1 and R2 are bound has such an oxidation potential that (1) the compound I has substantially no fluorescence before the cleavage; and (2) the resultant compound formed from I by the cleavage is substantially highly fluorescent after the cleavage.

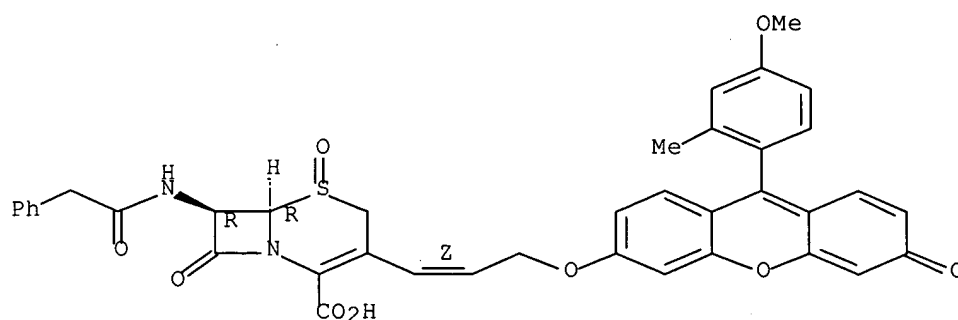
IT 847978-57-8P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (fluorescent probe capable of generating fluorescence upon bond cleavage in hydrolase assay)

RN 847978-57-8 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[(1Z)-3-[[9-(4-methoxy-2-methylphenyl)-3-oxo-3H-xanthen-6-yl]oxy]-1-propenyl]-8-oxo-7-[(phenylacetyl)amino]-, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:878473 HCAPLUS Full-text

DOCUMENT NUMBER: 141:389858

TITLE: reporting system for monitoring real-time gene expression events in live cells using fluorogenic substrates

INVENTOR(S): Xie, X. Sunney; Xiao, Jie; Cai, Long; Markson, Joseph Scott; Yu, Ji; Yin, Jialu

PATENT ASSIGNEE(S): President and Fellows of Harvard College, USA; Regents of the University of California

SOURCE: PCT Int. Appl., 69 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004090104	A2	20041021	WO 2004-US10341	20040402
WO 2004090104	A3	20050303		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1616032	A2	20060118	EP 2004-749716	20040402
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

PRIORITY APPLN. INFO.: US 2003-459897P P 20030402

WO 2004-US10341 W 20040402

AB The current invention provides a reporting system for monitoring real-time gene expression events in live cells using fluorogenic substrates. Modified β -galactosidase, β -glucosidase, β -lactamase with short maturation time and a short cellular lifetime are selected as reporter to detect transient gene

expression event in live cells. Gene expression signals are monitored by visible and UV spectrometry, and fluorometry.

IT 452280-30-7, CR 2

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

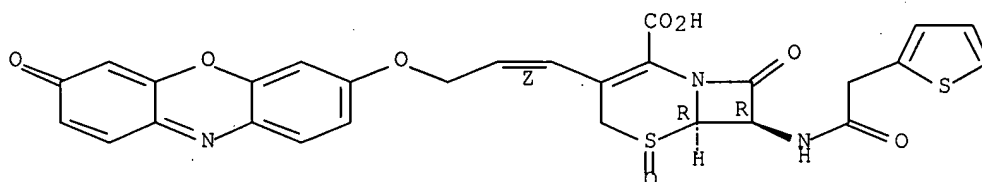
(CR 2; reporting system for monitoring real-time gene expression events in live cells using fluorogenic substrates)

RN 452280-30-7 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L61 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:643607 HCAPLUS Full-text

DOCUMENT NUMBER: 139:287990

TITLE: Novel Fluorogenic Substrates for Imaging β -Lactamase Gene Expression

AUTHOR(S): Gao, Wenzhong; Xing, Bengang; Tsien, Roger Y.; Rao, Jianghong

CORPORATE SOURCE: Department of Molecular and Medical Pharmacology, Crump Institute for Molecular Imaging, University of California, Los Angeles, CA, 90095-1770, USA

SOURCE: Journal of the American Chemical Society (2003), 125(37), 11146-11147

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:287990

AB A new class of small nonfluorescent fluorogenic substrates, based on release of a phenolic dye from a vinylogous cephalosporin, becomes brightly fluorescent after β -lactamase hydrolysis with up to 153-fold enhancement in the fluorescence intensity. Less than 500 fM of β -lactamase in cell lysates can be readily detected, and β -lactamase expression in living cells can be imaged with a red fluorescence derivative. These new fluorogenic substrates should find uses in clin. diagnostics and facilitate the applications of β -lactamase as a biosensor.

IT 609812-89-7P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(preparation of vinylogous cephalosporin fluorogenic substrates and use for detection of β -lactamase)

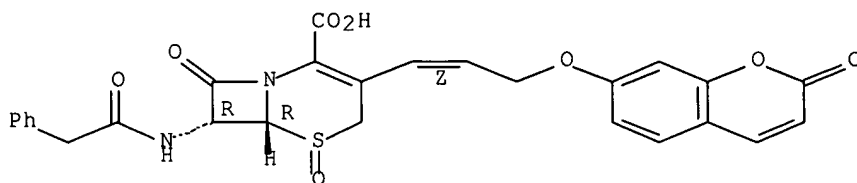
RN 609812-89-7 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 8-oxo-3-[(1Z)-3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-

[(phenylacetyl)amino]-, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:676218 HCAPLUS Full-text

DOCUMENT NUMBER: 137:197525

TITLE: β -Lactamase substrates having phenolic ethers and their use for β -lactamase determination

INVENTOR(S): Tsien, Roger Y.; Rao, Jianghong

PATENT ASSIGNEE(S): The Regents of the University of California, USA

SOURCE: PCT Int. Appl., 46 pp.

CODEN: PIXXD2

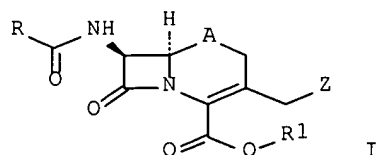
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002068678	A2	20020906	WO 2002-US769	20020111
WO 2002068678	A3	20031204		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2434679	A1	20020906	CA 2002-2434679	20020111
EP 1385853	A2	20040204	EP 2002-720779	20020111
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2005501806	T	20050120	JP 2002-568772	20020111
PRIORITY APPLN. INFO.:			US 2001-261313P	P 20010112
			WO 2002-US769	W 20020111
OTHER SOURCE(S):		MARPAT 137:197525		
GI				



AB Provided are fluorescent β -lactamase substrates I (R = benzyl, 2-thienylmethyl, cyanomethyl; R1 = H, physiologically acceptable salts or metal, ester groups, ammonium cations, --CHR2OCO(CH2)nCH3, --CHR2OCOC(CH3)3, acylthiomethyl, acyloxy- α -benzyl, δ -butyrolactonyl, methoxycarbonyloxymethyl, Ph, methylsulphinylmethyl, β -morpholinoethyl, dialkylaminoethyl, dialkylaminocarbonyloxymethyl; R2 = H, lower alkyl; A = S, O, SO, SO2, CH2; Z = a donor fluorescent moiety). Also provided are methods of use of these compounds for β -lactamase determination

IT 452280-30-7P 452280-31-8P 452280-32-9P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

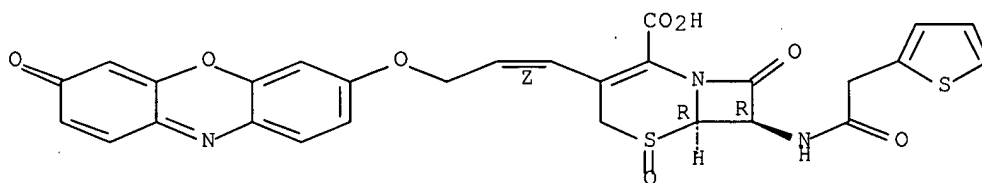
(β -Lactamase substrates having phenolic ethers and their use for β -lactamase determination)

RN 452280-30-7 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

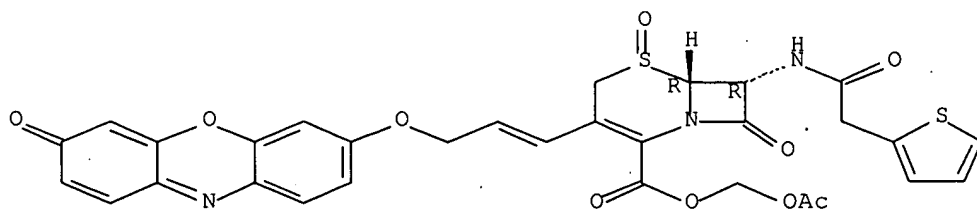


RN 452280-31-8 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 8-oxo-3-[3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, (acetyloxy)methyl ester, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

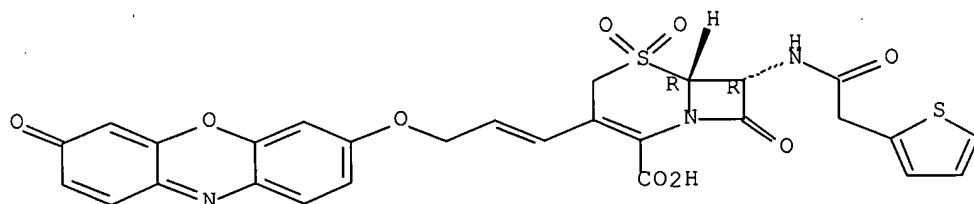


RN 452280-32-9 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
8-oxo-3-[3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-
thienylacetyl)amino]-, 5,5-dioxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.



HISTORY

=> d his nofil

(FILE 'HOME' ENTERED AT 13:54:44 ON 16 JAN 2007)

FILE 'REGISTRY' ENTERED AT 13:54:54 ON 16 JAN 2007

L1 STR
 L2 50 SEA SSS SAM L1
 L3 81306 SEA SSS FUL L1
 SAVE TEMP L3 BERCH019/A

FILE 'STNGUIDE' ENTERED AT 13:56:45 ON 16 JAN 2007

FILE 'REGISTRY' ENTERED AT 14:02:39 ON 16 JAN 2007

E CYANINE
 E CYANINE/CN
 L4 2 SEA ABB=ON PLU=ON CYANINE/CN
 D SCA
 L5 STR L1
 L6 50 SEA SUB=L3 SSS SAM L5
 L7 STR L5
 L8 STR L7
 L9 40 SEA SUB=L3 SSS SAM L8
 L10 706 SEA SUB=L3 SSS FUL L8
 L11 STR L8
 L12 587 SEA SUB=L10 SSS FUL L11
 L13 119 SEA ABB=ON PLU=ON L10 NOT L12
 L14 57 SEA ABB=ON PLU=ON L13 AND C6/ES
 L15 STR L8
 L16 0 SEA SUB=L10 SSS FUL L15
 L17 16 SEA ABB=ON PLU=ON L10 AND C6-C6/ES
 L18 16 SEA ABB=ON PLU=ON L17 AND S/ELS
 L19 9 SEA ABB=ON PLU=ON L17 AND S>1
 D SCA
 L20 1 SEA ABB=ON PLU=ON L13 AND NC4-C6/ES
 D SCA
 L21 6 SEA ABB=ON PLU=ON L13 AND N2C4-C6/ES
 D SCA
 L22 8 SEA ABB=ON PLU=ON L13 AND NC5-C6/ES
 D SCA
 L23 0 SEA ABB=ON PLU=ON L13 AND N2C3-N2C3/ES
 L24 0 SEA ABB=ON PLU=ON L13 AND NC5-C6-C6/ES
 L25 3 SEA ABB=ON PLU=ON L13 AND OC5-C6-C6/ES
 D SCA
 L26 6 SEA ABB=ON PLU=ON L13 AND OC5-C6/ES
 D SCA
 L27 0 SEA ABB=ON PLU=ON L26 AND NC5-C6-C6/ES
 L28 0 SEA ABB=ON PLU=ON L13 AND NC5-C6-C6/ES
 L29 11 SEA ABB=ON PLU=ON L13 AND NC2OC2-C6-C6/ES
 L30 1 SEA ABB=ON PLU=ON L13 AND NC4-C6/ES
 D SCA
 L31 0 SEA ABB=ON PLU=ON L13 AND OC4-C6/ES

FILE 'HCAPLUS' ENTERED AT 14:37:38 ON 16 JAN 2007

L32 24 SEA ABB=ON PLU=ON L12

FILE 'REGISTRY' ENTERED AT 14:38:11 ON 16 JAN 2007

L33 0 SEA ABB=ON PLU=ON L13 AND (EU OR TB)/ELS

FILE 'HCAPLUS' ENTERED AT 14:38:23 ON 16 JAN 2007

L34 1 SEA ABB=ON PLU=ON L20
L35 1 SEA ABB=ON PLU=ON L25
L36 3 SEA ABB=ON PLU=ON L26
L37 5 SEA ABB=ON PLU=ON L29

FILE 'HCAPLUS' ENTERED AT 14:39:32 ON 16 JAN 2007

D QUE L32
D L32 IBIB AB HITSTR TOT
D QUE L34
D QUE L35
D QUE L36
D QUE L37
L38 7 SEA ABB=ON PLU=ON (L34 OR L35 OR L36 OR L37)
D L38 IBIB ABS HITSTR TOT
D QUE L3
DIS

FILE 'REGISTRY' ENTERED AT 15:08:41 ON 16 JAN 2007

L39 STR L1
L40 STR L39
L41 4 SEA SUB=L3 SSS SAM L40
L42 40 SEA SUB=L3 SSS FUL L40

FILE 'HCAPLUS' ENTERED AT 15:15:59 ON 16 JAN 2007

L43 25 SEA ABB=ON PLU=ON L42

FILE 'REGISTRY' ENTERED AT 15:16:05 ON 16 JAN 2007

L44 27 SEA ABB=ON PLU=ON L42 AND C6/ES
D SCA
L45 0 SEA ABB=ON PLU=ON L42 AND NC5-C6-C6/ES
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L47 0 SEA ABB=ON PLU=ON L42 AND NC4-C6/ES
L48 0 SEA ABB=ON PLU=ON L42 AND NC5-C6/ES
L49 0 SEA ABB=ON PLU=ON L42 AND C6-C6/ES
L50 0 SEA ABB=ON PLU=ON L42 AND N2C3-N2C3/ES
L51 1 SEA ABB=ON PLU=ON L42 AND OC5-C6-C6/ES
D SCA
L52 2 SEA ABB=ON PLU=ON L42 AND OC5-C6/ES
D SCA
L53 5 SEA ABB=ON PLU=ON L42 AND NC2OC2-C6-C6/ES
L54 0 SEA ABB=ON PLU=ON L42 AND NC4-C6/ES
L55 0 SEA ABB=ON PLU=ON L42 AND OC4-C6/ES
L56 STR
L57 4 SEA SUB=L42 SSS FUL L56
D SCA

FILE 'HCAPLUS' ENTERED AT 15:25:55 ON 16 JAN 2007

L58 1 SEA ABB=ON PLU=ON L51
L59 3 SEA ABB=ON PLU=ON L52
L60 4 SEA ABB=ON PLU=ON L53

FILE 'HCAPLUS' ENTERED AT 15:26:16 ON 16 JAN 2007

D QUE L58
D QUE L59
D QUE L60
L61 6 SEA ABB=ON PLU=ON (L58 OR L59 OR L60)
D L61 IBIB ABS HITSTR TOT

L63 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:646444 HCAPLUS

DOCUMENT NUMBER: 137:361886

TITLE: Studies of lanthanide(III) metal complexes of
7-(D- α -aminophenylacetamido)-3-methyl-3-cephem-4-
carboxylic acid

AUTHOR(S): Pingalkar, S. R.; Deshpande, M. N.

CORPORATE SOURCE: P. G. Dep. of Chem., Science College, Nanded, 431 602,
IndiaSOURCE: Asian Journal of Chemistry (2002), 14(3-4), 1459-1462
CODEN: AJCHEW; ISSN: 0970-7077

PUBLISHER: Asian Journal of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:361886

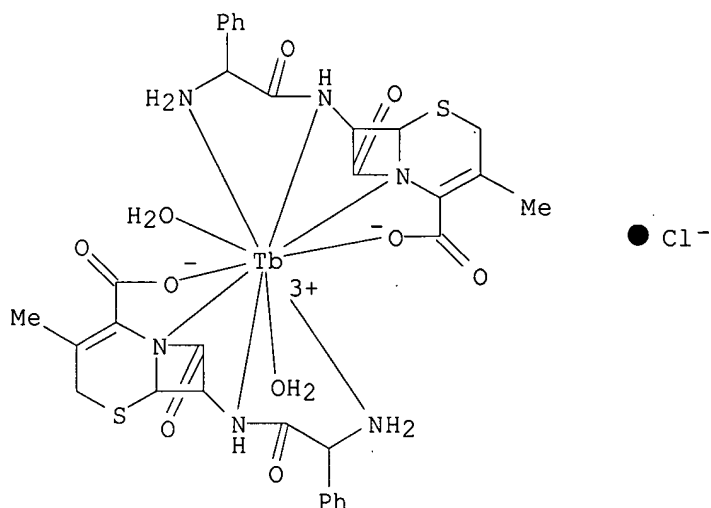
AB Eight new solid complexes of lanthanide(III) chlorides with
7-(D- α -aminophenylacetamido)-3-methyl-3-cephem-4-carboxylic acid
(AAMCC) were synthesized. These complexes are characterized by elemental
anal., UV (no data) and IR spectroscopies, magnetic moment, and solution
conductivity data. Corrosion inhibitory effect of these complexes and study of
antibacterial activity is also undertaken (no data). The IR spectral
studies indicate that the ligand acts as tetradentate and it coordinates
through amido, amino and ring N's and carboxylate O. The general formula
of the complexes is $[LnL_2(H_2O)_2]Cl$, where Ln = La(III), Ce(III), Pr(III),
Nd(III), Sm(III), Gd(III), Tb(III) and Dy(III) and L =
7-(D- α -aminophenylacetamido)-3-methyl-3-cephem-4-carboxylate. The
coordination number of the central metal ion is 10. An inhibitory study on
the corrosion of steel alloy in a solution of HNO₃ by the complexes was done.
Inhibitor concns. of 0.5 to 2% in 0.5 N HNO₃ were used, and inhibitory
efficiency increased in the order metal chloride < ligand < complex.
Antibacterial activity of AAMCC ligand increased upon complexation with
lanthanides (no data).

IT 474900-63-5P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); TEM
(Technical or engineered material use); BIOL (Biological study); PREP
(Preparation); USES (Uses)
(preparation, corrosion inhibitor activity of steel alloy in nitric acid,
and bactericidal activity of)

RN 474900-63-5 HCAPLUS

CN Terbium(1+), bis[7-[(amino- κ N)phenylacetyl]amino- κ N]-3-methyl-
8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylato-
 κ N1, κ O2]diaqua-, chloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L63 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:606991 HCAPLUS

DOCUMENT NUMBER: 131:225488

TITLE: Fluorogenic β -lactam preparation and β -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance

INVENTOR(S): Tsien, Roger Y.; Zlokarnik, Gregor

PATENT ASSIGNEE(S): The Regents of the University of California, USA

SOURCE: U.S., 58 pp., Cont. of U. S. Ser. No. 727,616.

CODEN: USXXAM

DOCUMENT TYPE: Patent

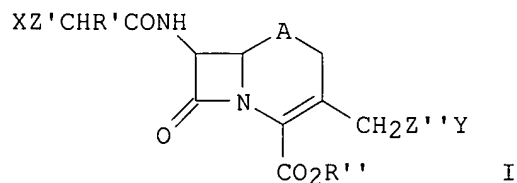
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5955604	A	19990921	US 1997-955401	19971021
US 6291162	B1	20010918	US 1996-727616	19961015
PRIORITY APPLN. INFO.:			US 1996-727616	A1 19961015
			US 1996-732178	A1 19961016
			US 1995-407544	A2 19950320
			WO 1996-US4059	W 19960320

OTHER SOURCE(S): MARPAT 131:225488
GI



AB Substrates for β -lactamase are provided of the general formula I in which one of X and Y is a fluorescent donor moiety and the other is a quencher (which may or may not re-emit); R' is selected from the group consisting of H, lower (i.e., alkyl of 1 to about 5 carbon atoms) and (CH₂)_nOH, in which n is 0 or an integer from 1 to 5; R" is selected from the group consisting of H, physiol. acceptable metal and ammonium cations, -CHR₂OCO(CH₂)_nCH₃, -CHR₂OCOC(CH₃)₃, acylthiomethyl, acyloxy- α -benzyl, δ -butyrolactonyl, methoxycarbonyloxymethyl, Ph, methylsulfinylmethyl, β -morpholinoethyl, dialkylaminoethyl, acyloxyalkyl, dialkylaminocarbonyloxymethyl and aliphatic, in which R₂ is selected from the group consisting of H and lower alkyl; A is selected from the group consisting of S, O, SO, SO₂ and CH₂; and Z' and Z" are linkers for the fluorescent donor and quencher moieties. Methods of assaying β -lactamase activity and monitoring expression in systems using β -lactamase as a reporter gene also are disclosed. Examples include Drosophila or zebrafish embryo transformation assays as well as animal cell glucocorticoid receptor-mediated or β -adrenergic receptor-mediated transcription assays.

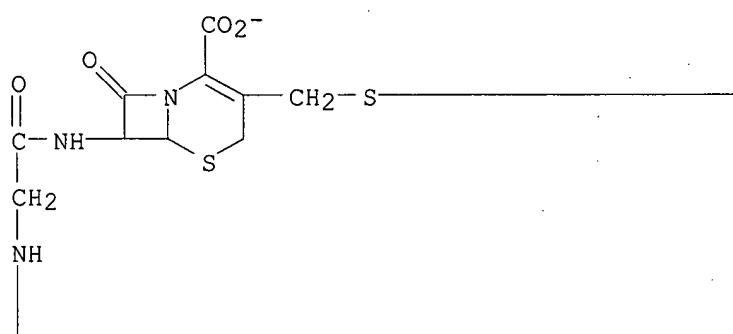
IT **183736-87-0**

RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)
(fluorogenic β -lactam preparation and β -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)

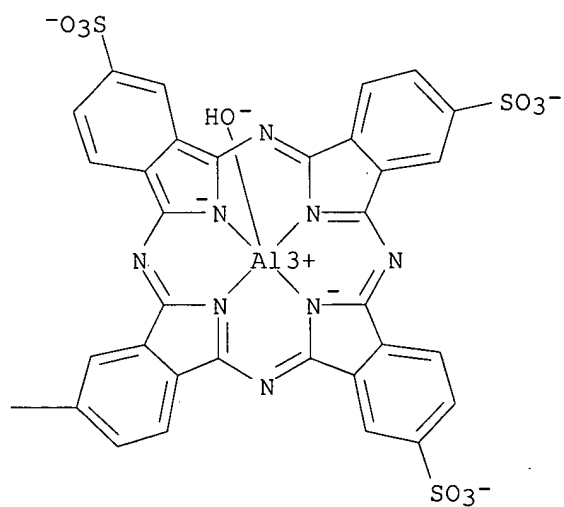
RN 183736-87-0 HCAPLUS

CN Europate(2-), [μ -[10-[[[2-[[2-carboxy-8-oxo-3-[[[9,16,23-trisulfo-29H,31H-phthalocyanin-2-yl]thio]methyl]-5-thia-1-azabicyclo[4.2.0]oct-2-en-7-yl]amino]-2-oxoethyl]amino]carbonyl]-1,14,39,40,41,42,43,44-octaazaocyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-5-carboxylato(8-)-N1,N14,N39,N40,N41,N42,N43,N44:N29,N30,N31,N32]](hydroxyaluminate)-(9CI) (CA INDEX NAME)

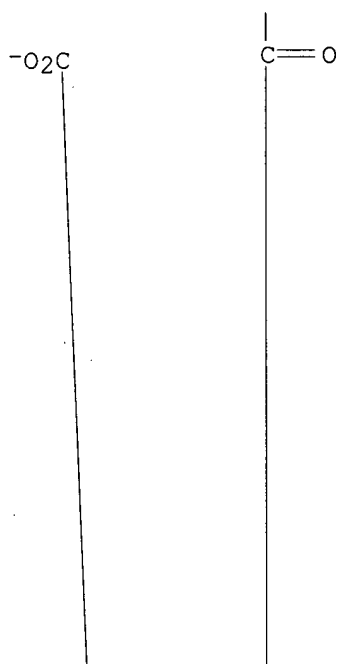
PAGE 1-A



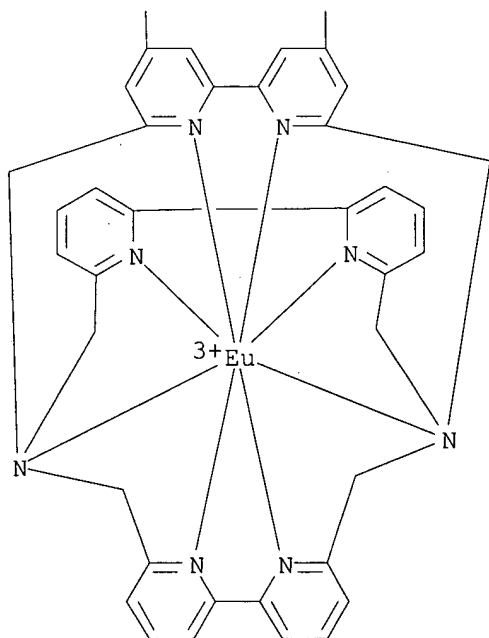
PAGE 1-B



PAGE 2-A



PAGE 3-A



REFERENCE COUNT: 83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L63 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:731813 HCAPLUS
 DOCUMENT NUMBER: 126:3785
 TITLE: Fluorogenic β -lactam preparation and
 β -lactamase reporter gene assay for animal cell
 transcription, transfection, or antibiotic resistance
 INVENTOR(S): Tsien, Roger Y.; Zlokarnik, Gregor
 PATENT ASSIGNEE(S): University of California, USA
 SOURCE: PCT Int. Appl., 118 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9630540	A2	19961003	WO 1996-US4059	19960320
WO 9630540	A3	19970109		
W:	AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI			
RW:	KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN			
US 5741657	A	19980421	US 1995-407544	19950320
CA 2215310	A1	19961003	CA 1996-2215310	19960320
CA 2215310	C	20020521		
AU 9655266	A	19961016	AU 1996-55266	19960320
AU 723164	B2	20000817		
EP 817785	A2	19980114	EP 1996-912454	19960320
EP 817785	B1	20010404		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
CN 1184479	A	19980610	CN 1996-193854	19960320
CN 1066731	B	20010606		
JP 11502714	T	19990309	JP 1996-529573	19960320
JP 3633940	B2	20050330		
AT 200287	T	20010415	AT 1996-912454	19960320
ES 2156994	T3	20010801	ES 1996-912454	19960320
AT 253632	T	20031115	AT 1999-118473	19960320
PT 982398	T	20040227	PT 1999-118473	19960320
EP 1405922	A2	20040407	EP 2003-25361	19960320
EP 1405922	A3	20040929		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
ES 2209305	T3	20040616	ES 1999-118473	19960320
US 6291162	B1	20010918	US 1996-727616	19961015
EP 982398	A1	20000301	EP 1999-118473	19990917
EP 982398	B1	20031105		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI			
US 6472205	B1	20021029	US 2000-481756	20000111
CN 1296078	A	20010523	CN 2000-122761	20000808
US 2003119085	A1	20030626	US 2002-280482	20021024
US 7157575	B2	20070102		
JP 2005021172	A	20050127	JP 2004-305450	20041020
JP 3856807	B2	20061213		
PRIORITY APPLN. INFO.:			US 1995-407544	A2 19950320
			EP 1996-912454	A3 19960320

JP 1996-529573	A3 19960320
WO 1996-US4059	W 19960320
US 1996-727616	A1 19961015
EP 1999-118473	A3 19990917
US 2000-481756	A1 20000111

OTHER SOURCE(S): MARPAT 126:3785

AB Fluorogenic β -lactam substrates are useful for detecting expression of the reporter gene, β -lactamase gene. Synthetic β -lactamase substrates with a fluorescent donor moiety in addition to a quencher moiety (which may or may not re-emit) are prepared and characterized. Synthetic substrates may include groups which are alkyl of 1 to about 5 carbon atoms or $(CH_2)_nOH$, in which n is 0 or an integer from 1 to 5. Synthetic substrates also may include physiologically acceptable metal and ammonium cations, $-CHR_2OCO(CH_2)_nCH_3$, $-CHR_2OCOC(CH_3)_3$, acylthiomethyl, acyloxy- α -benzyl, δ -butyrolactonyl, methoxycarbonyloxymethyl, Ph, methylsulphinylmethyl, β -morpholinoethyl, dialkylaminoethyl, acyloxyalkyl, and dialkylaminocarbonyloxymethyl groups. S, O, SO, SO₂ and CH₂ as well as linkers for the fluorescent donor and quencher moieties are also included in synthetic β -lactamase substrates. Methods of assaying β -lactamase activity and monitoring expression in systems using β -lactamase as a reporter gene also are disclosed. Examples include Drosophila or zebrafish embryo transformation assays as well as animal cell glucocorticoid receptor-mediated or β -adrenergic receptor-mediated transcription assays.

IT 183736-87-0

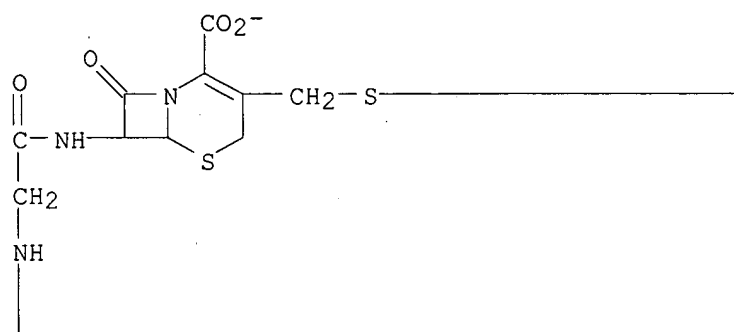
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)

(fluorogenic β -lactam preparation and β -lactamase reporter gene assay for animal cell transcription, transfection, or antibiotic resistance)

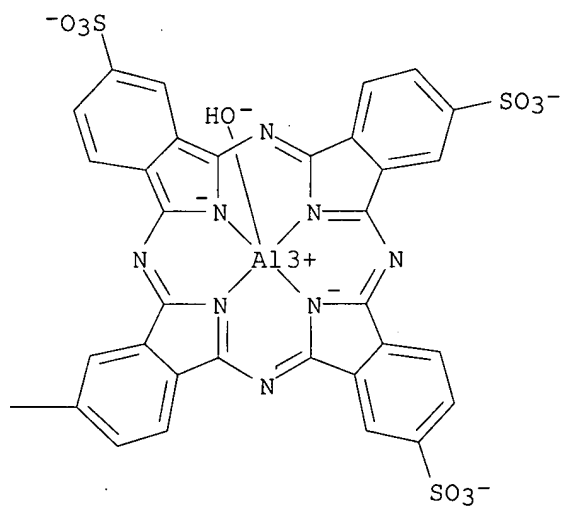
RN 183736-87-0 HCAPLUS

CN Europate(2-), [μ -[10-[[[2-[[2-carboxy-8-oxo-3-[[[9,16,23-trisulfo-29H,31H-phthalocyanin-2-yl]thio]methyl]-5-thia-1-azabicyclo[4.2.0]oct-2-en-7-yl]amino]-2-oxoethyl]amino]carbonyl]-1,14,39,40,41,42,43,44-octaazaoctacyclo[12.12.12.13,7.18,12.116,20.121,25.128,32.133,37]tetratetraconta-3,5,7(44),8,10,12(43),16,18,20(42),21,23,25(41),28,30,32(40),33,35,37(39)-octadecaene-5-carboxylato(8-)-N1,N14,N39,N40,N41,N42,N43,N44:N29,N30,N31,N32]](hydroxyaluminate)-(9CI) (CA INDEX NAME)

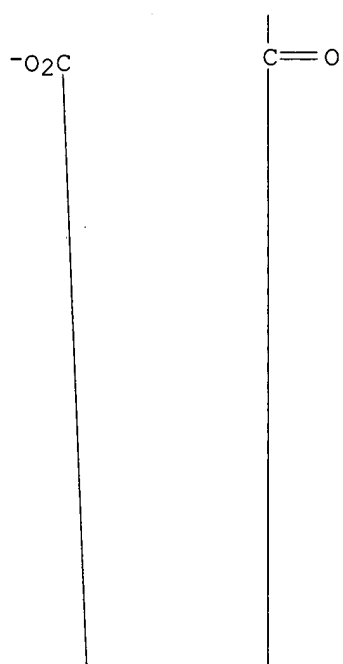
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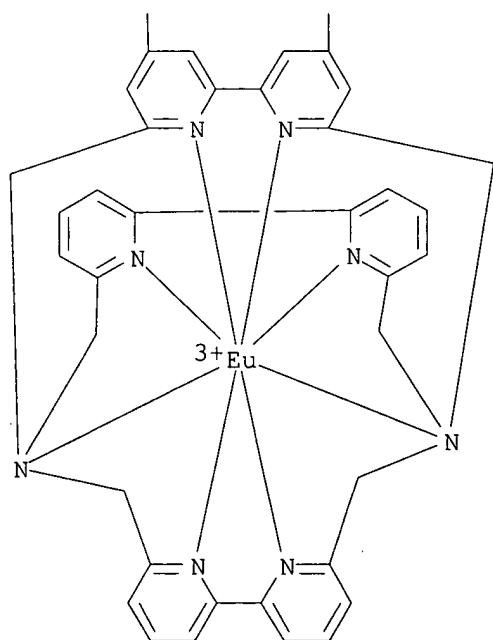
PAGE 1-B



PAGE 2-A

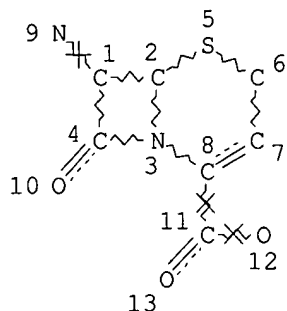


PAGE 3-A



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L1

STR



NODE ATTRIBUTES:

CONNECT IS M3 RC AT 7
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L3 81306 SEA FILE=REGISTRY SSS FUL L1
 L62 3 SEA FILE=REGISTRY ABB=ON PLU=ON L3 AND (EU OR TB)/ELS
 L63 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L62